Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 478 °C

Global applicability domain: Outside

Local applicability domain index: 3.06e-02

Confidence level: 3.87e-01

Nearest Neighbors from the Training Set

Image not found
Aminotrimethylene phosphonic
acid
Measured: 480
Predicted: 478

Image not found
Pentanedioic acid
Measured: 303
Predicted: 310

Image not found
Hexanedioic acid
Measured: 338
Predicted: 330

Image not found
Heptanedioic acid
Measured: 342
Predicted: 332

Image not found
Octanedioic acid
Measured: 346
Predicted: 332